Global Calculation of Nuclear Shape Isomers

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To determine which nuclei may exhibit shape isomerism, we use a well-benchmarked macroscopic-microscopic model to calculate potential-energy surfaces as functions of spheroidal (ϵ_2), hexadecapole (ϵ_4), and axial-asymmetry (γ) shape coordinates for 7206 nuclei from $A = 31$ to $A = 290$. We analyze these and identify the deformations and energies of all minima deeper than 0.2 MeV. These minima may correspond to characteristic experimentally observable *shape-isomeric* states. Shape isomers mainly occur in the $A = 80$ region, the $A = 100$ region, and in an extended region centered around ^{208}Pb. We compare our model to experimental results for Kr isotopes. Moreover, in a plot versus N and Z we show for each of the 7206 nuclei the calculated number of minima. The results reveal one fairly unexplored region of shape isomerism, which is experimentally accessible, namely the region northeast of $^{208}_{82}$Pb.

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The nuclear potential energy, calculated as a function of shape parameters may have several local minima. The lowest minimum is associated with the mass and shape of the nucleus. Additional minima are shape isomers and in even-even nuclei are manifested as excited 0^+ states, see Refs. [1–3]. Nuclear shape isomerism has previously been studied both experimentally and theoretically [4,5]. However, there has been no global study of shape isomers in a theoretical model with demonstrated predictive power which is universal and free of parameters specifically adjusted to shape-isomer data. Examples of previous, limited studies are in the reviews [4,5]. A typical example using the macroscopic-microscopic approach is in [6]. A more recent study with self-consistent Skyrme forces shows substantial sensitivity of the results to the particular force used [7]. Many studies have been performed without considering axial asymmetry; however, this is essential. Potential-energy surfaces obtained in most calculations limited to axially symmetric shapes will, for deformed nuclei, exhibit at least one prolate and one oblate ‘‘minimum’’. However, it is well known, and discussed in, for example [8], that most ‘‘shape isomers’’ obtained in such restricted calculations become unstable with respect to axial asymmetry when this constraint is removed.

In our study we consider axial asymmetry and present for the first time a global calculation of the occurrence of shape isomers in a model that describes nuclei from very light (normally ^{16}O) to the heaviest nuclei with a consistent set of parameters for all studied properties and all nuclei. The potential-energy surfaces are calculated in the macroscopic-microscopic finite-range liquid-drop model (FRLDM) with the recent 2002 parameter set [9]. It has been very extensively benchmarked and been shown to have excellent extrapolateability [10,11]. This is a ‘‘zero-order’’ approximation; it shows which nuclei fulfill a necessary condition for shape isomers, namely, the presence of multiple minima in the potential-energy surfaces. More elaborate models base a calculation of low-lying level energies on the detailed structure of the potential and go beyond the mean field by constructing wave functions in some type of mixing model [12–15]. However, despite our model simplicity, we obtain a good overlap between calculated regions of multiple minima and regions of experimentally observed shape coexistence. A complete description of the model used here and discussions of its key results can be found in [10,11,16,17].

To locate possible shape-isomer nuclei globally we calculate for 7206 nuclei from $A = 31$ to $A = 290$ the energy in a three-dimensional grid in terms of three deformation parameters, namely, quadrupole ϵ_2, hexadecapole ϵ_4, and axial asymmetry γ [8,18]. The grid is $\varepsilon_2 = (0.0, 0.025, \ldots, 0.45)$, $\gamma = (0.0, 2.5, \ldots, 60.0)$, and $\varepsilon_4 = (-0.12, -0.10, \ldots, 0.12)$, with altogether 6175 grid points. Our surfaces are identical to those used in our previous studies of ground-state axial asymmetry [8,18] and some additional details specific to the calculation of these surfaces can be found there. The omission of higher shape degrees of freedom such as ϵ_3 and ϵ_6 is not expected to be serious; they only affect a small percentage of all nuclei, and then normally to a small degree, see Figs. 14 and 19 in [10].

We show in Fig. 1 our results for $^{72}_{36}$Kr, the ‘‘poster child’’ of nuclear shape isomers. The ground state is oblate with $\varepsilon_2 = 0.35$ and $\gamma = 60$, but a prolate shape isomer 0.6 MeV above the ground state, with $\varepsilon_2 = 0.275$ is also present. The two minima are separated by a saddle at

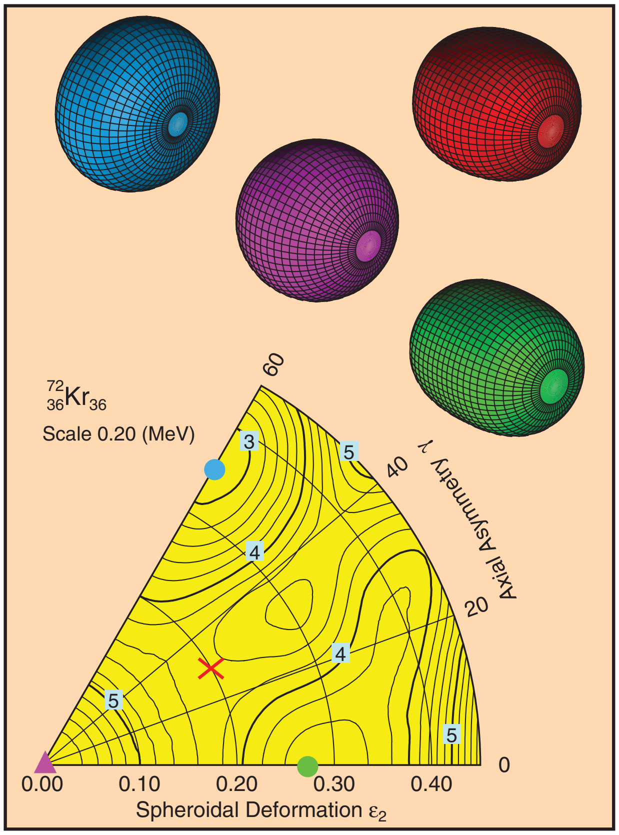

FIG. 1 (color). Calculated potential-energy surface for ^{72}Kr versus ε_2 and γ (minimized with respect to ε_4 [17]). The numbers on a blue background give the energy in MeV of the thicker contour lines which are spaced 1 MeV apart; the spacing between the thinner lines is 0.2 MeV. The circular arcs starting at $\epsilon_2 = 0.10$, 0.20, 0.30, and 0.40 and the straight lines ending at $\gamma = 20$ and 40 indicate the coordinate grid. To obtain a suitable range of values we have, following standard practice, subtracted the energy obtained for a spherical shape in the macroscopic part of the model. The lower left tip of the pie-like plot corresponds to a sphere (at energy 6.0 MeV). Points along the upper straight line correspond to oblate shapes (like a discus) and those along the lower straight line to prolate shapes (like an American football). The energy values in the interior are calculated for axially-asymmetric nuclear shapes (a somewhat simplified analogy is that these points correspond to shapes that result from standing on a football). Shapes corresponding to the oblate minimum (cyan-filled circle), the prolate minimum (green-filled circle), the saddle separating these two minima (crossed red lines), and to the sphere (magenta-filled triangle) are shown at the top in the colors of the symbols at their respective locations in the contour plot.

$\varepsilon_2 = 0.2$ and $\gamma = 30$ rising about 0.8 MeV above the prolate isomer minimum. The potential energy for $^{180}_{80}$Hg in Fig. 2 exhibits four minima, whereas the surface for $^{186}_{82}$Pb in Fig. 3 has five minima.

Spectroscopic studies of neutron-deficient nuclei for $A \sim 80$ give rich information about nuclear shape isomers. Shape isomers occur due to the competition between shapes polarized by the occupation of different orbits.

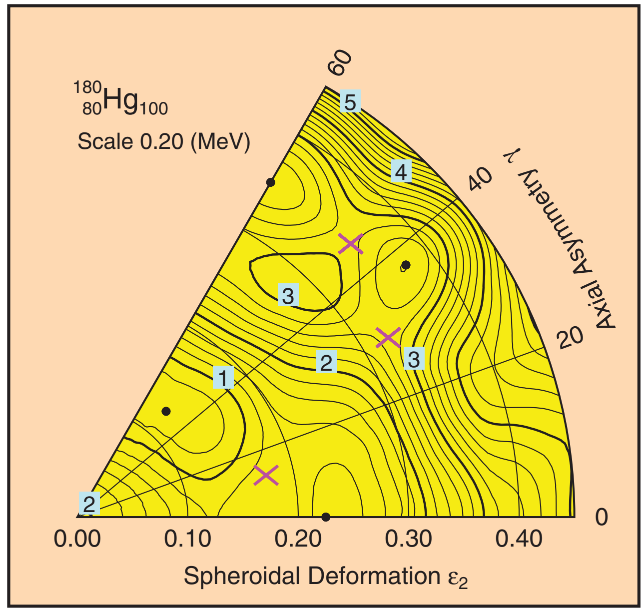

FIG. 2 (color). Calculated potential-energy surface versus ε_2 and γ for ^{180}Hg. Minima are shown as black dots, optimal saddles between pairs of minima as crossed lines. There are 4 minima. It is an interesting conjecture, which we at this point are not able to prove generally, that the number of saddle points needed to define optimal paths between n minima is $n - 1$, not $n \times (n - 1)/2$. Thus, our immersion method only identifies 3 optimal saddle points in this surface, rather than 6.

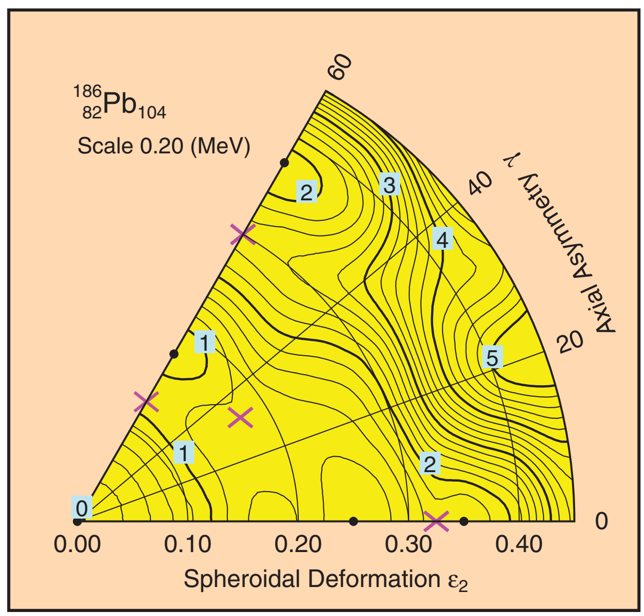

FIG. 3 (color). Calculated potential-energy surface versus ε_2 and γ for ^{186}Pb. There are 5 minima and 4 optimal saddle points in this surface. "Triple" shape isomers have been observed experimentally in this nucleus. In Fig. 5 only 4 minima are shown for this nucleus, because the minimum at $\epsilon_2 = 0.35$, $\gamma = 0$, is too shallow to be counted.

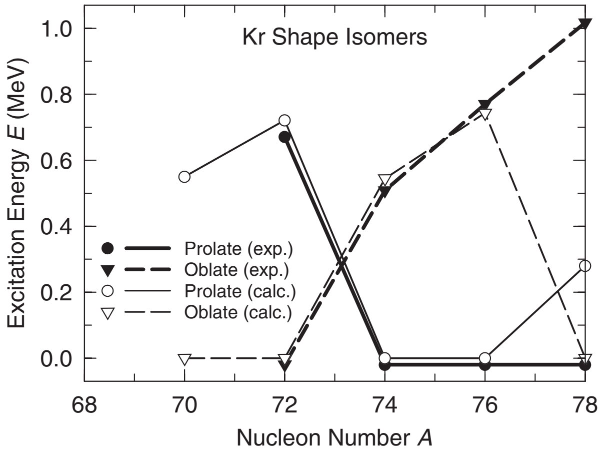

FIG. 4. Calculated energies and shapes (oblate or prolate) of the nuclear ground state and of the first excited 0^+ state compared to experimental data. See text for further discussions.

Competing are oblate (34,36,40), spherical (38,40) and prolate (34,38,40) shell gaps. Normally the deformed gaps "win" over the spherical gaps. Therefore ground states correspond to deformed oblate or prolate shapes in this region. Spherical minima, if they exist, are a couple of MeV higher in energy. Because of the coexisting shell gaps, adding or removing just a few nucleons can have a dramatic effect on the nuclear shape in nuclei with $A \sim 80$. The simultaneous occurrence of prolate, oblate, and spherical minima is also expected in a single nucleus for a few favorable cases.

One of the fingerprints of shape isomers in even-even nuclei is low-lying excited 0^+ states, which are often interpreted as a signature of a shape that is different from the ground-state nuclear shape. In neutron-deficient Kr isotopes, excited 0^+ states are consistently observed below $E_x = 1$ MeV in ^{72}Kr [3], ^{74}Kr [19] and ^{76}Kr [20]. In all the isotopes, a regular rotational band is observed for spins $I > 6\hbar$, while the regularity is missing in the lower angular-momentum states $I \leq 6\hbar$. These irregularities of the low-energy spectra of the Kr isotopes can be understood in terms of the prolate-oblate shape isomers, with both minima exhibiting large deformations, approximately $|\epsilon_2| = 0.3$–0.4. In another experiment and related theoretical studies [14], data for ^{74}Kr and ^{76}Kr confirm the prolate shape in the ground-state bands and the opposite sign of the intrinsic Q moments of 2_2^+ and 2_3^+ which can be

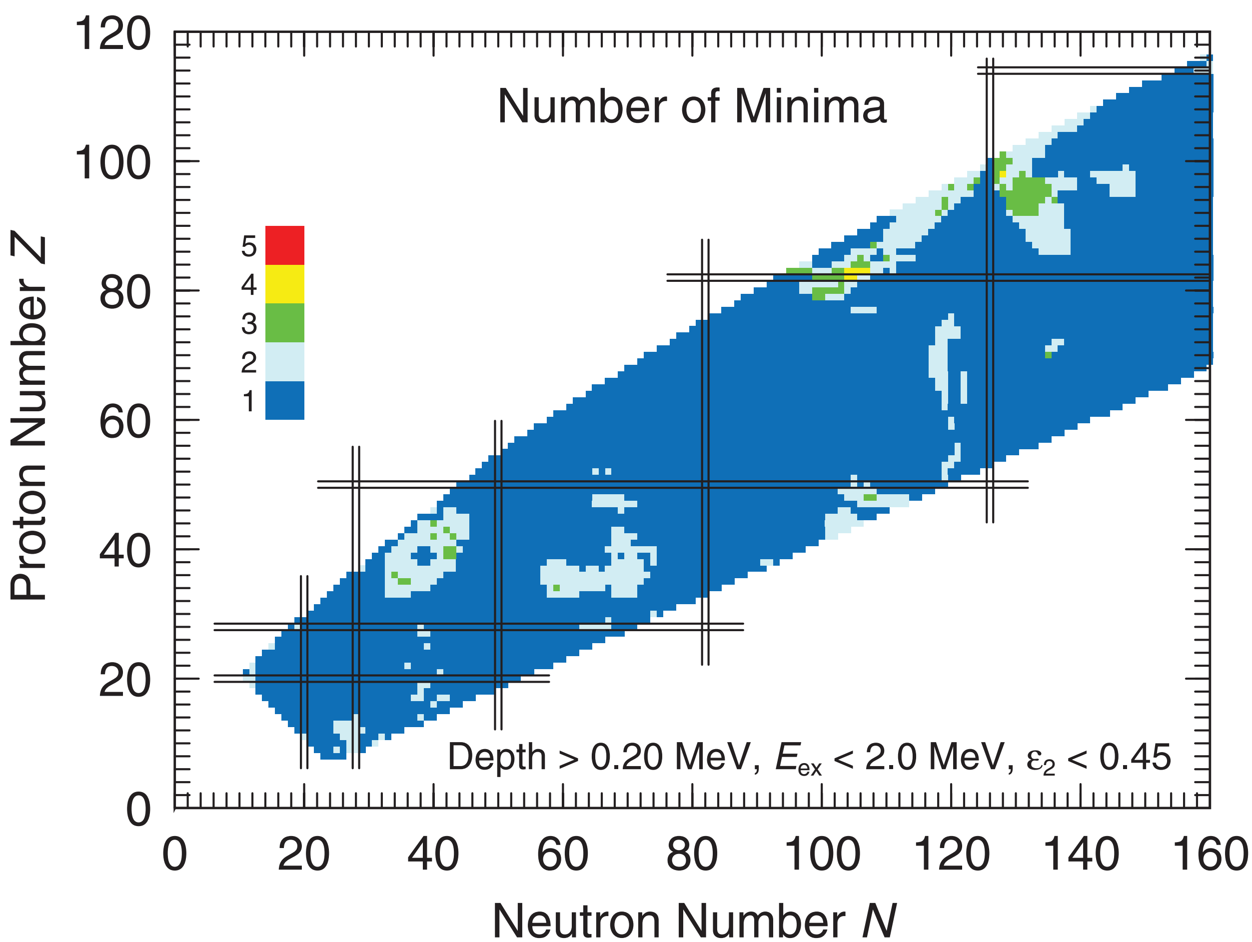

FIG. 5 (color). Number of minima found with deformation $\epsilon_2 < 0.45$. Only the ground-state and isomer minima that are deeper than 0.2 MeV and with energies relative to the ground state of less than 2.0 MeV are counted.

interpreted as the evidence of either an oblate shape or a γ vibration.

We show the calculated results for the lowest two 0^+ configurations in the Kr isotopes in Fig. 4. All prolate and oblate minima obtained in our 3D calculation have been further minimized in a 4D space [21]. The ground states of ^{70}Kr and ^{72}Kr have oblate shapes with $|\epsilon_2| = 0.325$–0.350 and the prolate minima are found at 600–800 keV higher energies than the oblate minima. On the other hand, in ^{74}Kr and ^{76}Kr, the lowest minima are prolate with $|\epsilon_2| \sim 0.350$ and the oblate minima are found around 600 keV higher than the prolate minima. The theoretical results on this isotope sequence are remarkably consistent with the experimental observations on shape isomers in the Kr isotopes, except for ^{78}Kr. For this isotope our calculated isomer minimum is less than 0.2 MeV, deep, and should not be counted according to our rule not to count minima shallower than 0.2 MeV. It also has a triaxial deformation of $\gamma = 17.5$. In Ref. [3] it is suggested that an extrapolation procedure based on higher-energy members of rotational bands can provide "unperturbed" energies of the 0^+ states and our results agree somewhat less well with these energies. However, sophisticated studies of shape isomers in models beyond mean field, for example [22,23] reproduce the oblate-prolate shifts in the ground-state deformations less well than our model. In contrast, other studies have been more successful [12,13].

Triple shape isomers have been observed in $^{186}_{82}$Pb with energies of the two excited 0^+ states at 0.532 MeV (oblate) and 0.650 MeV (prolate). Our calculated minima at 0.8 and 1.1 MeV would correspond to these experimental observations.

While an in-depth analysis of our complete results will be published elsewhere, we conclude by summarizing our results on shape isomers in Fig. 5 in which we show the number of minima for each nuclide in terms of a contour diagram versus N and Z. For shape isomers to be counted their excitation energy has to be below 2 MeV, their deformation less than $\varepsilon_2 = 0.45$, and their depth larger than 0.2 MeV. By depth we mean that the saddles between the minimum considered and lower minima all have to be higher than 0.2 MeV with respect to the energy of that minimum. Other criteria are obviously possible, but we feel that this choice would reveal isomer minima that may have observable experimental signatures. The saddle between two minima is determined by an immersion technique described in [16] and in more extensive detail in [17]. We find that shape isomers in nuclei that can be studied experimentally are roughly limited to the neutron-deficient $A \approx 80$, neutron-rich $A \approx 100$, neutron-deficient Pb, and neutron-deficient actinide regions. Based on our results here the little-studied neutron-deficient actinide region could be a "new continent" awaiting exploration.

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